

Se-(8-Azidoadenosyl)selenomethionine

135608-83-2 | DTXSID70159478

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 174 °C

Global applicability domain: Outside

Local applicability domain index: 1.58e-01

Confidence level: 7.06e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Famotidine</div> <div>Measured: 164</div> <div>Predicted: 171</div>	<div>Image not found</div> <div>Thiamine disulfide</div> <div>Measured: 177</div> <div>Predicted: N/A</div>	<div>Image not found</div> <div>Puromycin</div> <div>Measured: 176</div> <div>Predicted: 176</div>
<div>Image not found</div> <div>Psicofuranine</div> <div>Measured: 212</div> <div>Predicted: 215</div>	<div>Image not found</div> <div>Deferoxamine</div> <div>Measured: 140</div> <div>Predicted: 142</div>	